# Universality of temperature-dependent effects in finite many-fermion systems

O. Civitarese
*Departamento de Física, Universidad de la Plata, CC 67 (1900) La Plata, Argentina*

G. G. Dussel*
*Departamento de Física, Facultad de Ciencias Exactas y Naturales, Ciudad Universitaria, Nuñez 1428, Buenos Aires, Argentina, and Laboratoire de Physique Nucléaire Théorique, Centre de Recherche Nucleaire, Strasbourg, France*

A. P. Zuker
*Laboratoire de Physique Nucléaire Théorique, Centre de Recherche Nucleaire, Strasbourg, France*

(Received 19 July 1989)

The temperature dependence of the specific heat for a finite system of fermions is investigated for some simple models. It is found that finite-size effects produce a maximum in the specific heat at a temperature $T_c$ that has a universal value when scaled by the appropriate characteristic energy.

The study of temperature-dependent properties in finite nuclei has been the subject of different approaches[1–6] that rely mainly on the validity of the mean field approximation[7] and assume that the validity of standard methods of quantum statistical mechanics extends to such small systems, although there is evidence of deviations due to their finite size.[8]

It is our purpose to study the most schematic model that could shed light on two aspects of the problem: the finite number of particles and the finite size of the Hilbert space in which they evolve (even if there are many of them). The first aspect is related to the equivalence of canonical and grand canonical descriptions (a necessary condition for the latter to make sense in a mean field approach as usually assumed). The second aspect does not concern the validity of statistical mechanics but the type of thermodynamics it produces; in particular the appearance of a maximum in the specific heat that seems to point to some general behavior in a bound system of fermions. In what follows, whenever we use the terms "bound" or "finite size" it should be understood they apply to the energy bound and to the quantized Hilbert or Fock space. The small number of particles will turn out to be of little consequence in our models.

Consider $N$ particles distributed over two shells separated by an energy $D$, each having degeneracy $2M$. The number of states that can be constructed by putting $n$ particles in one of the shells is the combinatorial number $\binom{2M}{n}$. The partition function for the canonical ensemble (CE) is then

$$Z_N^{\mathrm{CE}}=\sum_{n=0}^{N}\binom{2M}{n}\binom{2M}{N-n}e^{-nD/T}\,, \tag{1}$$

where we have assumed the lowest shell to be at energy 0. For $M=\frac{1}{2}$, $N=1$, $Z_N$ coincides with the well-known problem of independent spins[9] ($S$ from now on). Since the sum in (1) becomes trivial, it is very easy to calculate the mean energy $(E)$ and specific heat $(C)$ by taking derivatives of $Z_1$ with respect to $1/T$ in the standard way. For larger values of $N$ the calculation can be done numerically, and Fig. 1 shows the aspect of $C(T)$ for several values of $N=2M$. It is seen that the appearance of a maximum for the $S$ system (the Schottky effect) is a common feature for all values of $N$. From this we conclude that the maximum is not associated with the small number of particles, but with the small number of shells. Indeed, if we do the $N=1$ calculation for an harmonic spectrum (i.e., an infinite number of equidistant levels) we obtain

$$Z_{\mathrm{HO}}=e^{-D/2T}\sum_{n=0}^{\infty}e^{-nD/T}=\frac{1}{2\sinh(D/2T)}\,, \tag{2}$$

which yields a specific heat that has no maximum (Fig. 1).

In the grand canonical ensemble (GCE), strict conservation of the number of particles is replaced by an average conservation

$$\begin{aligned} Z_N^{\mathrm{GCE}}&=\sum_N e^{\lambda N}Z_N^{\mathrm{CE}}\\ &=\sum_{n_i}\binom{2M_1}{n_1}e^{-n_1(\varepsilon_1-\lambda)/T}\binom{2M_2}{n_2}e^{-n_2(\varepsilon_2-\lambda)/T}\cdots\\ &=\prod_i\left(1+e^{-(\varepsilon_i-\lambda)/T}\right)^{2M_i}\,, \end{aligned} \tag{3a}$$

$$\langle N\rangle=\frac{1}{Z_N^{\mathrm{GCE}}}\frac{\partial Z^{\mathrm{GCE}}}{\partial\lambda}=\sum_i\langle n_i\rangle=N\,. \tag{3b}$$

This general form, valid for an arbitrary family of shells of energies $\varepsilon_i$ and degeneracies $2M_i$, is easier to write than to handle because of condition (3b). However, for $N=2M_1=2M_2=2M$ we find, by symmetry, $\lambda=0$, $\varepsilon_1=-\varepsilon_2=-D/2$, and the occupancy of the shells becomes

$$\begin{aligned} n_1&=n_{\mathrm{lower}}=N(1+e^{-D/2T})^{-1}\,,\\ n_2&=n_{\mathrm{upper}}=N(1+e^{D/2T})^{-1}\,, \end{aligned} \tag{4}$$

 

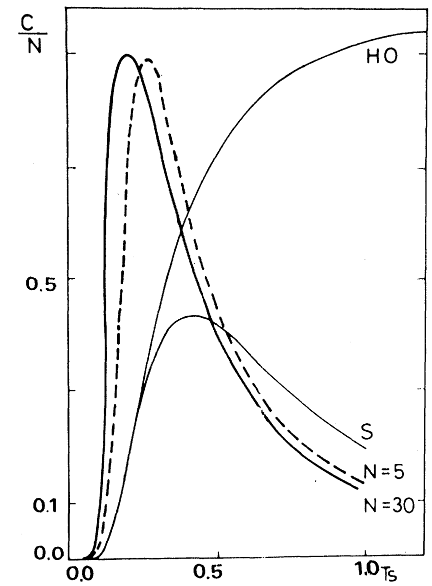


FIG. 1. Specific heat per particle $C/N$ as a function of the scaled temperature $T_s = T/D$. The curves denoted by HO and $S$ correspond to the harmonic oscillator and spin systems, respectively. The curves denoted by $N=5$ and 30 are the results obtained in the CE for these two values of $N=2M$.

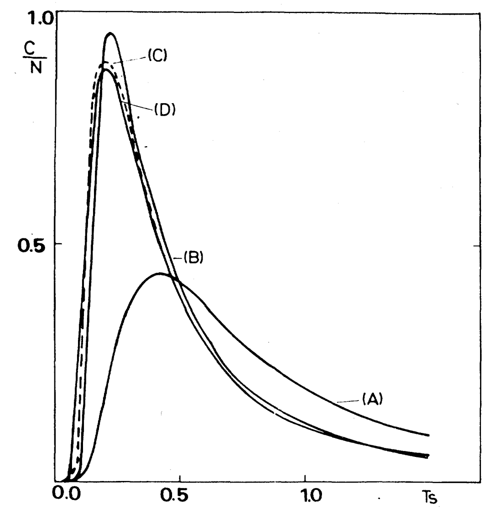


FIG. 2. Specific heat per particle $C/N$ as a function of $T_s = T/D$ for the CE [(A), (B), and (C)] and the GCE [(D)]. The curves denoted by (A), (B), and (C) correspond to $2M=N=1$, 10, and 40, respectively.

from which we have

$$E = -\frac{D}{2}(n_1 - n_2) = -\frac{DN \sinh x}{2(1+\cosh x)} ,$$
$$C = \frac{Nx^2}{1+\cosh x} , \quad (5)$$
$$x = D/(2T) .$$

The specific heat has a maximum at $x_c$, such that

$$x_c \sinh x_c - 2\cosh x_c = 2 , \quad (6)$$

which yields $x_c = 2.40$ or $T_s^c = 0.208$.

The subscript $s$ stands for "scaled." Figure 2 compares several CE results with the GCE one [Eq. (3)], and it is evident that for all intents, for $N \gtrsim 5$ the thermodynamics of both descriptions coincide (a reassuring result).

Other two-shell calculations with $2M_1 = N$, $2M_2 = 10^k M$ have been done. The form of $\lambda$ is nontrivial but simple. The peak of the specific heat increases by a factor $O(k)$ while $T_s^c$ is reduced by a factor $O(1/k)$ (Hardy's order notation).

We obtain the following general result: A system of $N$ particles moving in two shells separated by an energy $D$ and having a total degeneracy of $O(2N)$ has a peak in $C$ for the scaled temperature $T_s^c \simeq 0.20$. Before examining the consequences of this result, we consider the effects of truncation in a continuous distribution.

We have calculated the specific heat for a degenerate Fermi gas system, where the momentum distribution is given by

$$\rho(\xi) = 1/\{1+\exp[(\xi^2 - \mu/\varepsilon_F)/T_s]\} \quad \xi \le q$$
$$= 0, \quad \xi > q$$

where $\xi = k/k_F$; $T_s = T/\varepsilon_F$; and $k_F$ ($\varepsilon_F$) being the Fermi momentum (energy) at $T=0$.

For this scaled distribution the chemical potential $\mu/\varepsilon_F$ is determined by imposing the conservation of the number of particles, i.e.,

$$\int_0^\infty \rho(\xi)\xi^2 d\xi = \tfrac{1}{3} ,$$

and the specific heat per particle is given by

$$\frac{C}{N} = \frac{4}{3T_s^2}\int_0^\infty \rho(\xi)\xi^4 \left[\xi^2 - \frac{\mu}{\varepsilon_F}\right] \exp\left[\left[\xi^2 - \frac{\mu}{\varepsilon_F}\right] \Big/ T_s\right] d\xi .$$

The results obtained for $C/N$ are shown in Fig. 3 for different values of the cutoff $q$. It has a maximum for a scaled critical temperature $T_s^c$ that increases linearly with $q$. The maximum value of the specific heat also increases almost linearly with $q$. For reasonable values of $q$, $T_s^c$ varies between 0.15 and 0.35, thus giving support to the ideas that finite-size effects are responsible for the appearance of a peak in the specific heat in this range of values of $T_s$.

We can summarize the results obtained in the simple models studied as follows:

(a) The appearance of a peak in the specific heat for a system of noninteracting particles is related to the existence of a bound in the energy of the single-particle spectrum.

(b) To the extent a bound system [in the sense of (a)]

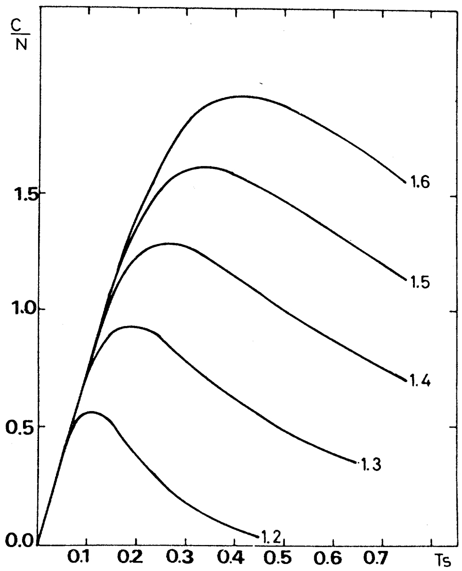


FIG. 3. Specific heat per particle for the truncated Fermi gas, for different values of the cutoff momentum $q$.

can be characterized by a single energy parameter $E_c$, its specific heat shows a peak at $T_s^c = T/E_c \simeq 0.20$.

Although the results of the calculation for the two-shell case are strongly limited by the schematic nature of the model space, the main features which emerge from them are similar to those found for the truncated Fermi gas calculations. Therefore, some attention has to be paid to finite-size effects which are not determined by the dynamical response of finite fermionic systems at nonzero temperatures but by the finite dimensional structure of them.

For the simple systems we have studied $C$ goes to zero at $T=0$ *and* $T=\infty$, as the energy cannot increase indefinitely with $T$. This is a sufficient condition for the existence of a maximum, but not a necessary one. If we compare curves $S$ and HO in Fig. 1, or the different curves in Fig. 3, we see that at low $T$, $C$ is not affected by the bound in energy, but as soon as it is, the maximum comes very fast. A similar behavior could obtain if instead of a sudden cutoff in the spectrum we had a dramatic increase in the density of states. In that case we should extend our notion of "bound system" and we could even expect a true singularity rather than a mere bump, as hinted at in the second paragraph after Eq. (6). Be as it may, there seems to be a hint that at $T_s^c = 0.2$ some sort of transition must take place for bound systems of fermions that is not dictated by details of their dynamics but by finite-size effects. Let us examine some examples.

(i) *Superconductivity.* The characteristic energy is, for the paired fermions, of the order of $2\Delta$, $\Delta$ being the value of the pairing gap. Therefore, we would expect to find a transition to the unpaired states at $T_c \simeq 0.4\Delta$. This result agrees well with the corresponding values for finite[10] as well as for infinite[11] systems, where $T_c \simeq 0.5\Delta$.

(ii) *Shells in a central potential.* The shell corrections are associated with the energy differences between a uniformly distributed spectra and nonuniform one. For a heavy system, like $^{208}$Pb, $E_c \simeq 7$ MeV, i.e., the energy gap between major shells. In this case one obtains $T_c \simeq 1.4$ MeV, which is in good agreement with the theoretical estimates of 1.7 MeV for the temperature associated with the collapse of shell effects obtained in Ref. 12.

(iii) *Fermions in the nuclear central potential.* In this case, $E_c = E_F$ (the Fermi energy) = 40 MeV. In consequence, one obtains $T_c \simeq 8$ MeV, in remarkable agreement with the average separation energy for a nucleon.

(iv) *Shape transitions in deformed nuclei.* In this case,[13] the characteristic energy is 16 MeV for the transition from prolate to spherical shape, while its value is 12 MeV for the oblate to spherical situation. The corresponding values for $T_c$ are 3.2 MeV and 2.8 MeV, and therefore $T_s^c = 0.20$ and 0.23, respectively.

(v) *Quarks in a nucleon.* If we assume as characteristic energy the nucleon rest mass, of the order of 1 GeV, the critical temperature associated with the transition to the deconfined phase would be of the order of 200 MeV, a value which is consistent with the estimates (Ref. 14) of quantum chromodynamics (QCD).

One is tempted to speculate that the type of universality obtained for the critical temperature $T_s^c$ that we have found is just another manifestation of the universal behavior found at $T=0$ for composite systems formed by many fermions.[15]

We would like to thank Lutz Dohnert and James Vary for helpful discussions and comments. This work was supported in part by Carrera del Investigador Cíentifico, CONICET, Argentina.

---

*On leave from Departamento de Física, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina.

[1]A. L. Goodman, Nucl. Phys. **A352**, 30 (1981); **A352**, 45 (1981); **A369**, 365 (1981); **A370**, 90 (1981); **A406**, 94 (1983); **A402**, 189 (1983).

[2]D. Vautherin and N. Vinh Mau, Phys. Lett. **120B**, 261 (1983); Nucl. Phys. **A422**, 1 (1984).

[3]M. Barranco, A. Polls, and J. Martorell, Nucl. Phys. **A444**, 445 (1985).

[4]O. Civitarese, C. Dasso, and R. A. Broglia, Ann. Phys. (N.Y.) **156**, 142 (1984).

[5]O. Civitarese and A. L. De Paoli, Nucl. Phys. **A440**, 480 (1985).

[6]M. Brack and P. Quentin, Nucl. Phys. **A361**, 35 (1981).

[7]D. J. Thouless, *The Quantum Mechanics of the Many Body Systems* (Academic, New York, 1961).

[8]K. Binder, J. Comput. Phys. **59**, 1 (1985).

[9]J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (Wiley, New York, 1940), especially Sec. 6i.
[10]O. Civitarese, G. G. Dussel, and R. P. J. Perazzo, Nucl. Phys. **A404**, 15 (1983).
[11]A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1963), especially Chap. 7, p. 296.
[12]O. Civitarese and A. L. De Paoli, Z. Phys. A **350**, 317 (1983).
[13]H. G. Miller, R. M. Quick, G. Bozzolo, and J. P. Vary, Phys. Lett. **168B**, 13 (1986); in *Condensed Matter Theories,* edited by F. B. Malik (Plenum, New York, 1986), p. 165.
[14]*Quick Matter Formation and Heavy Ion Collisions, Proceedings of the Bielefield Workshop, 1982,* edited by M. Yacov and H. Satz (World Scientific, Singapore, 1982).
[15]J. H. Rose, J. P. Vary, and J. R. Smith, Phys. Rev. Lett. **53**, 344 (1984).